

# Using Machine Learning for spin-group reclassification of neutron resonances

G.P.A. Nobre<sup>1</sup>, D. Brown<sup>1</sup>, S. Hollick<sup>2</sup>, S. Scoville<sup>3</sup>, P. Rodriguez<sup>4</sup>,  
M. Fucci<sup>5</sup>, R.-M. Crawford<sup>6</sup>, S. Ruiz<sup>7</sup>, A. Coles<sup>1</sup>, M. Vorabbi<sup>1</sup>

<sup>1</sup>National Nuclear Data Center, Brookhaven National Laboratory,

<sup>2</sup>Yale University, Physics Department,

<sup>3</sup>Rensselaer Polytechnic Institute, Department of Physics,

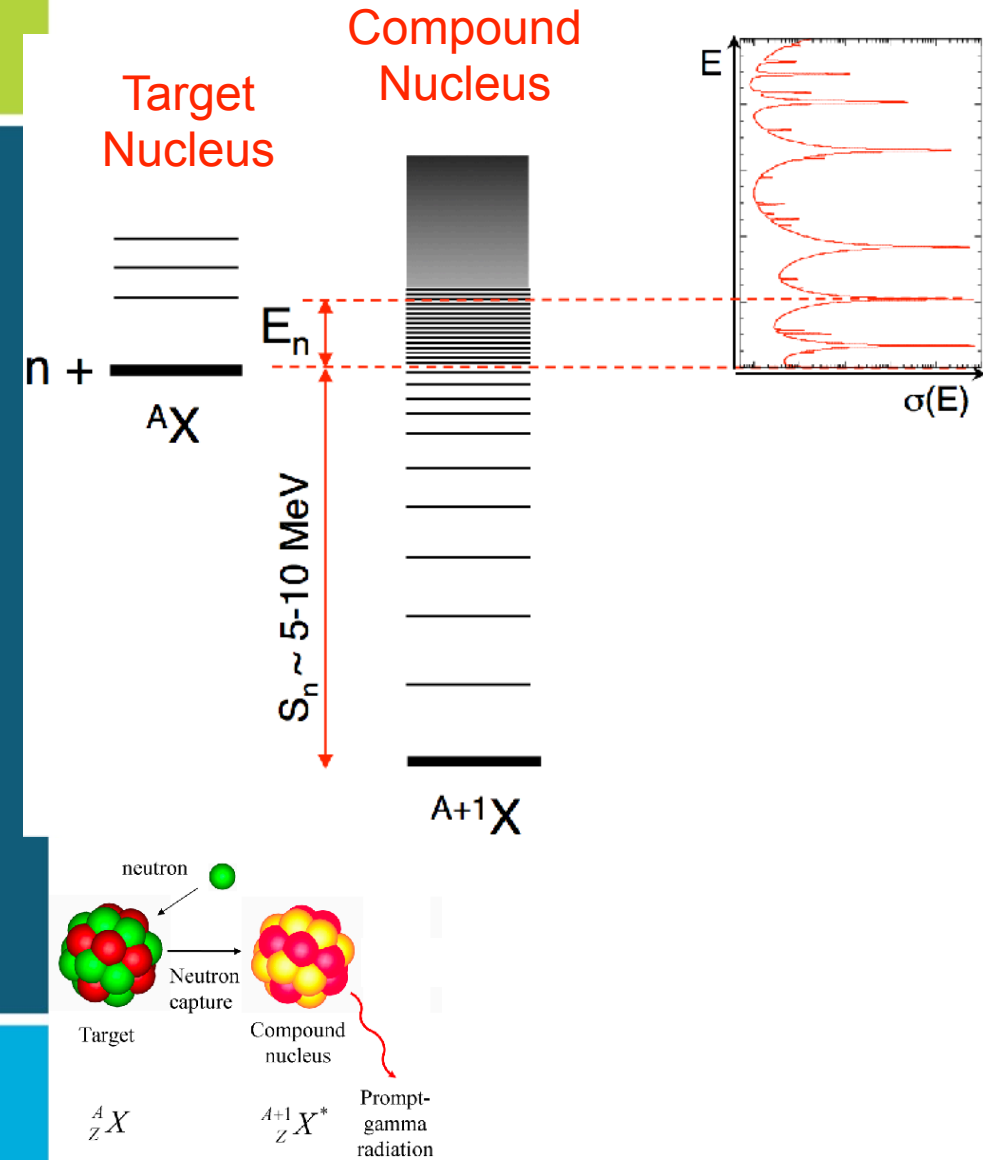
<sup>4</sup>University of Puerto Rico, Mayagüez Campus,

<sup>5</sup>University At Albany, Department of Physics,

<sup>6</sup>Willamette University, Department of Physics,

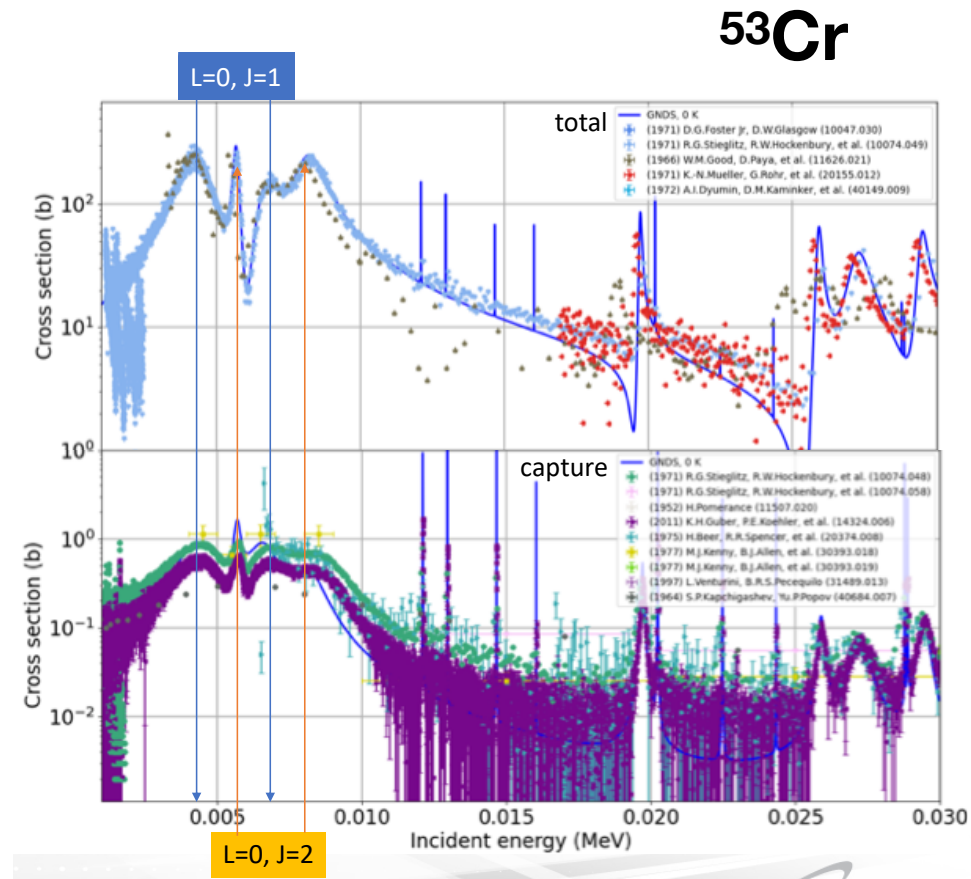
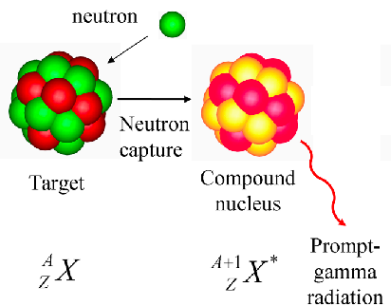
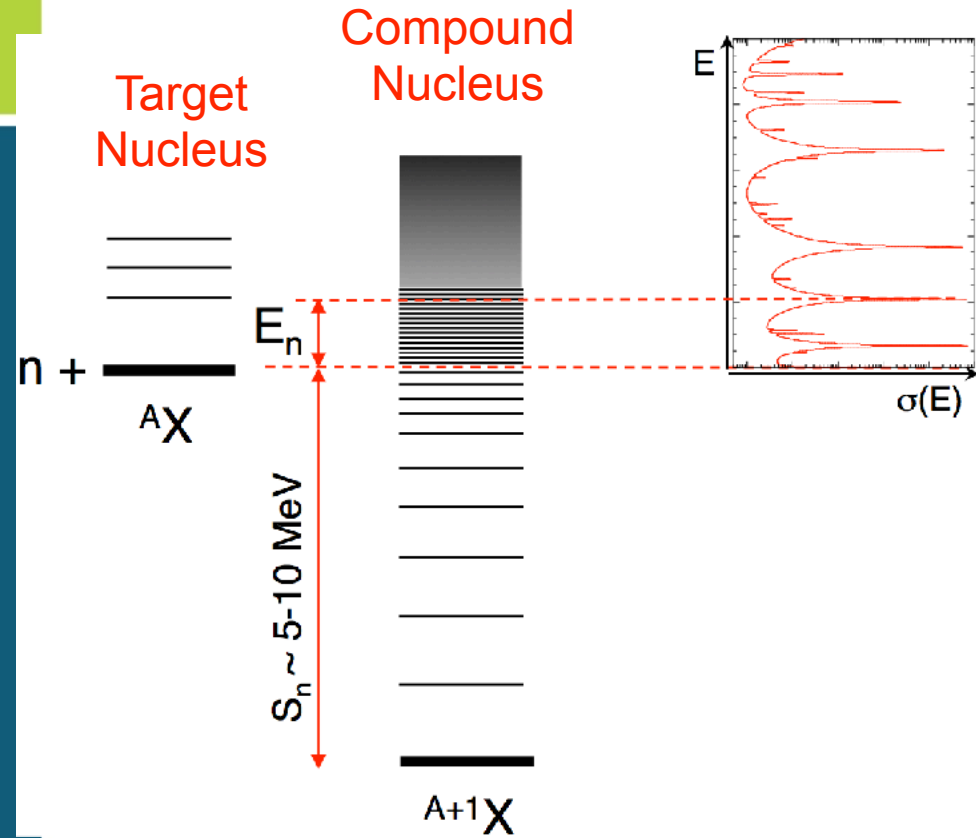
<sup>7</sup>Georgia Institute of Technology, School of Physics

# What are neutron resonances?

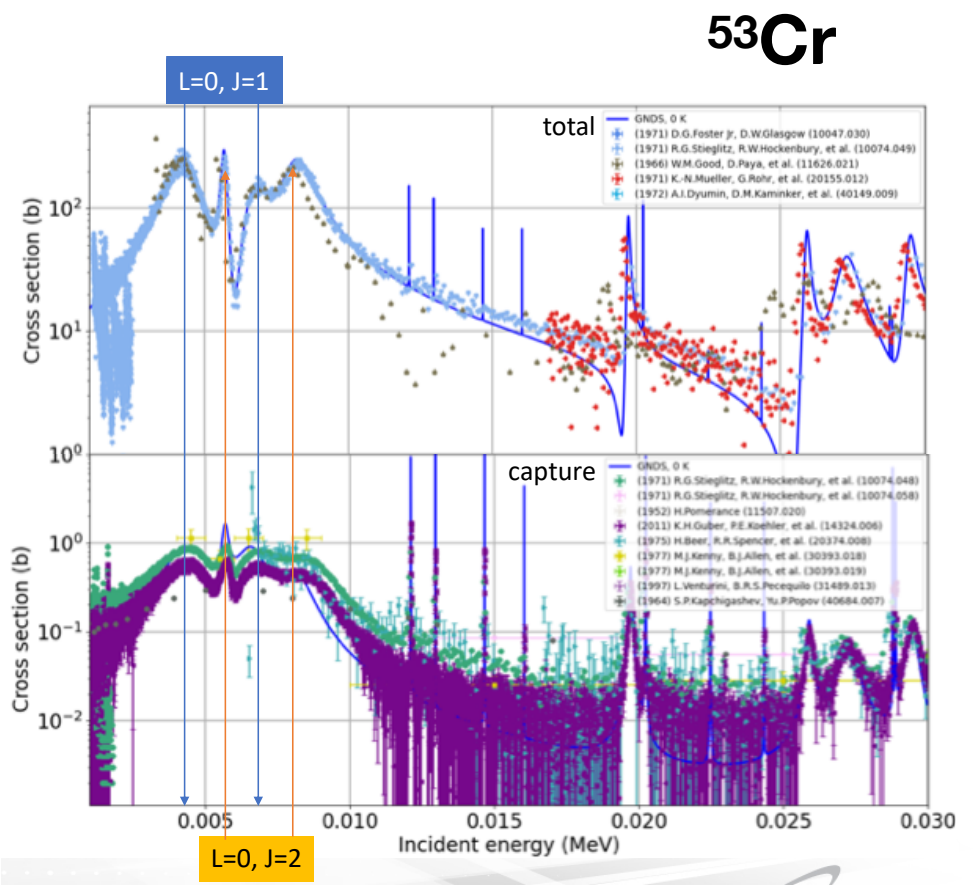
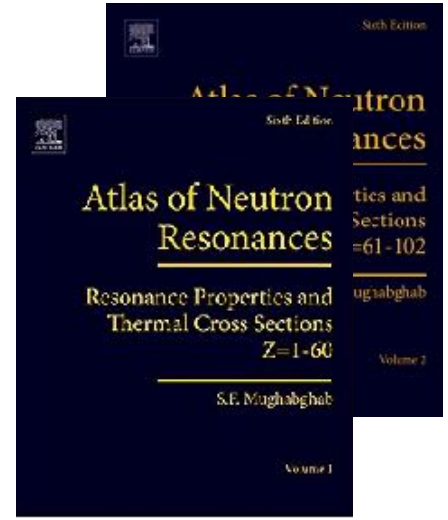
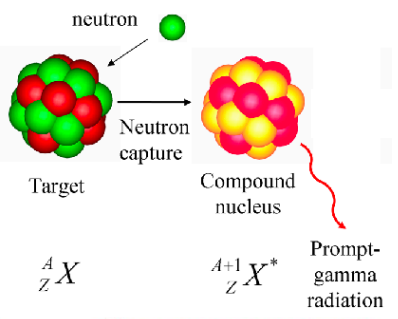
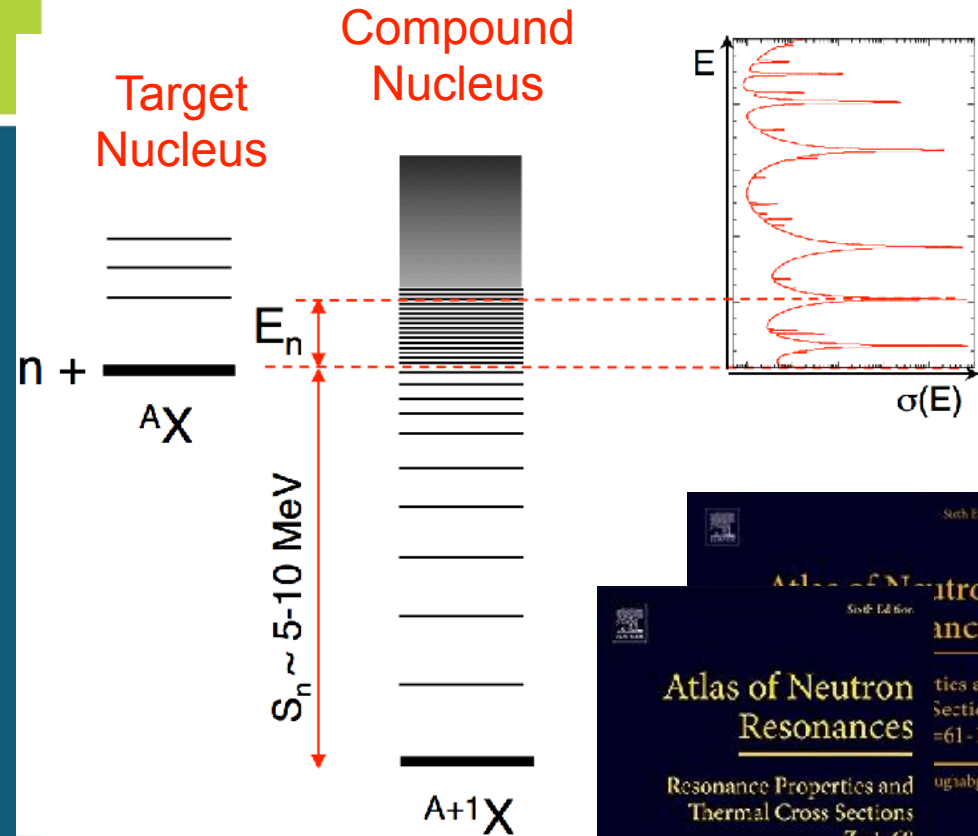




# What are neutron resonances?

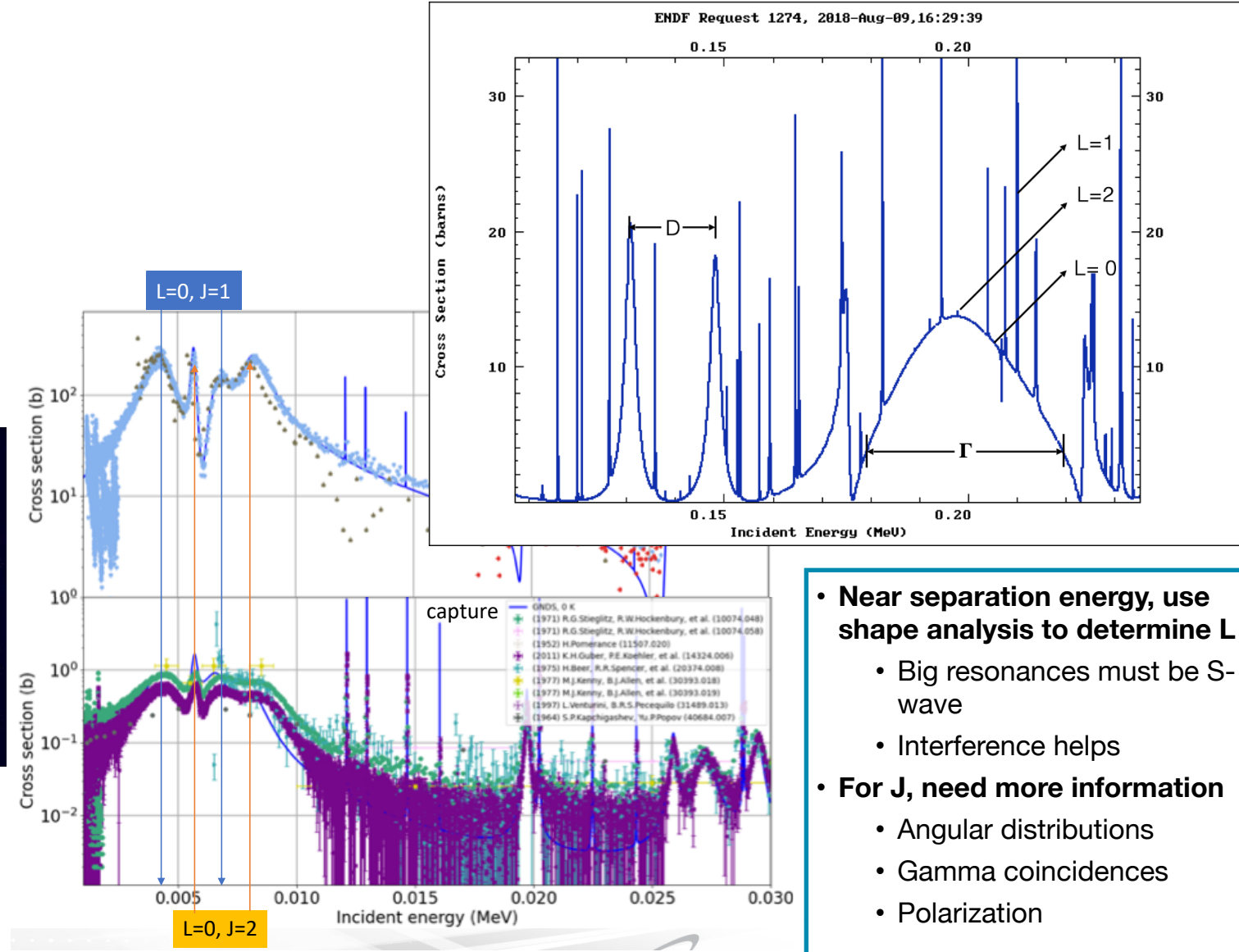
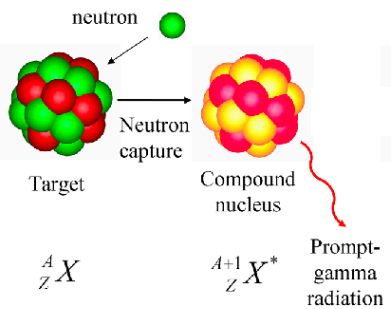
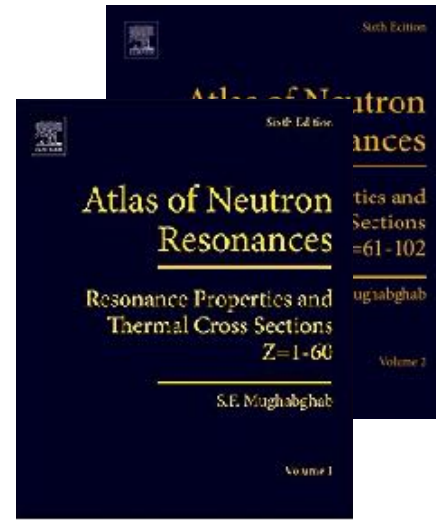
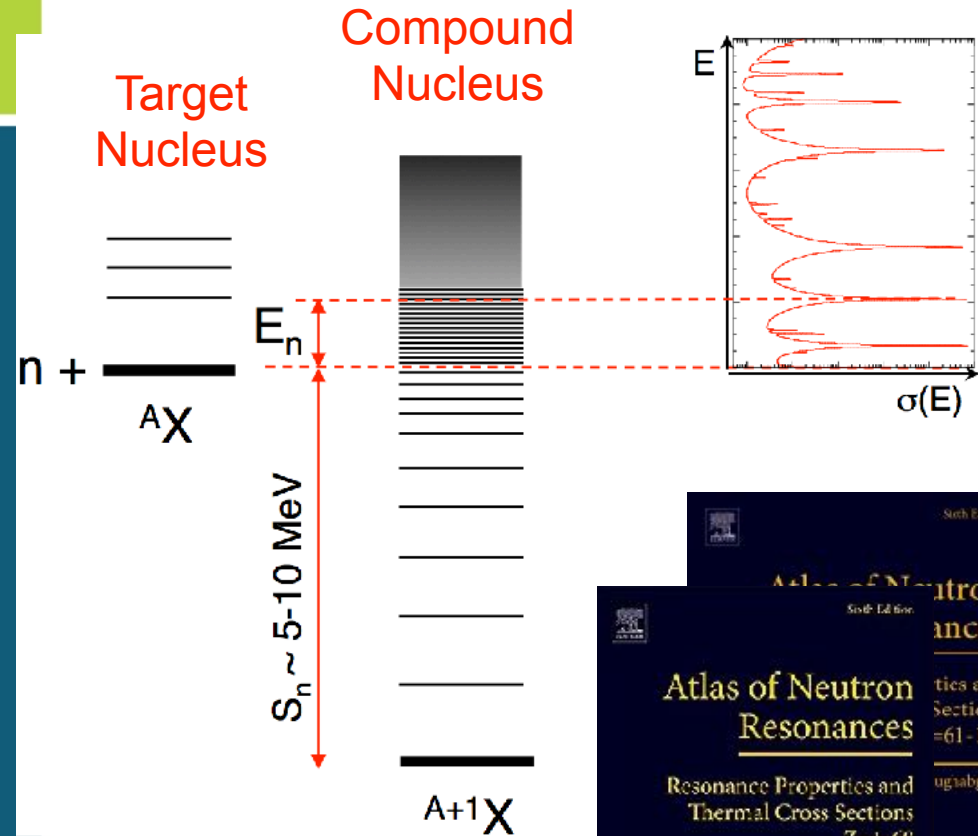


# What are neutron resonances?





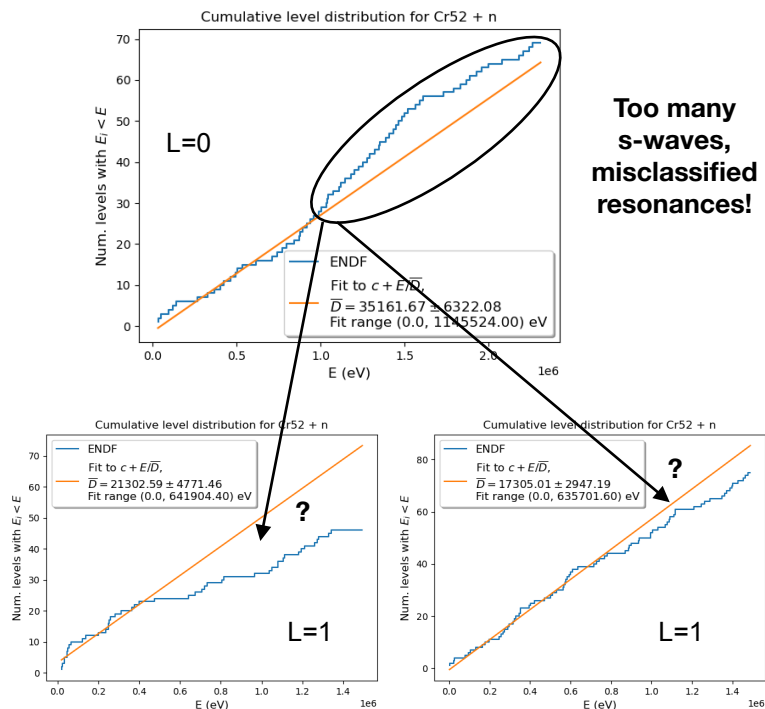
# What are neutron resonances?



- Near separation energy, use shape analysis to determine L
  - Big resonances must be S-wave
  - Interference helps
- For J, need more information
  - Angular distributions
  - Gamma coincidences
  - Polarization

# Identifying resonance spin assignments is tricky

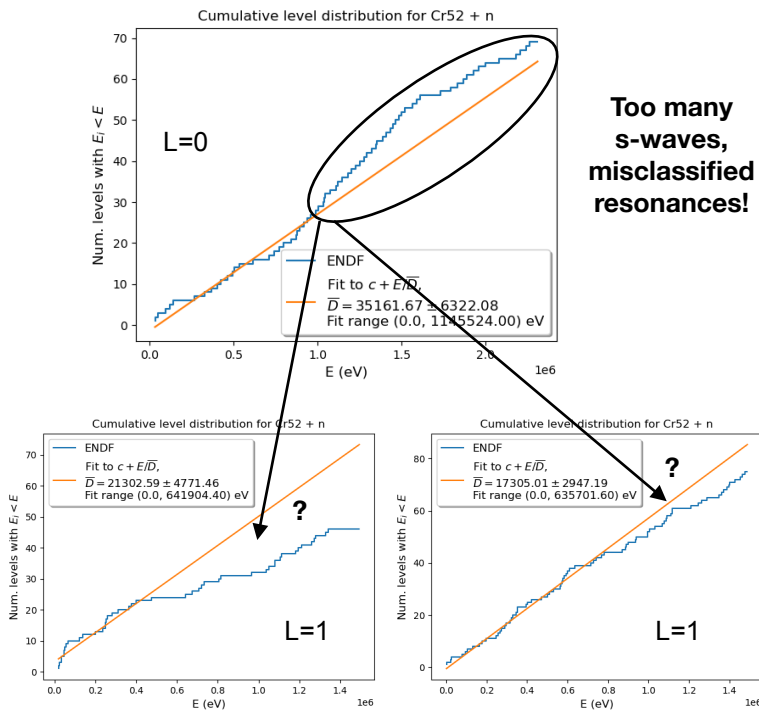
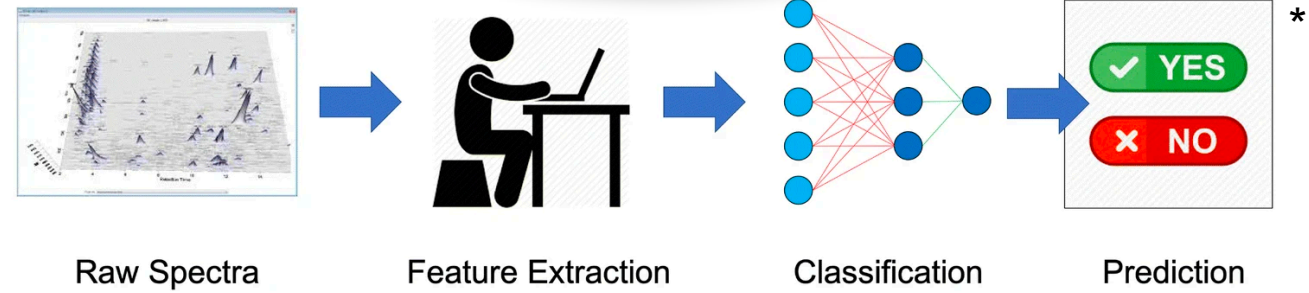
- Process of fitting R-matrix to data can be difficult, time consuming and may not be reproducible
- The Atlas is rife with misclassified resonances!
- Often done with trial, error and significant human intervention



# Identifying resonance spin assignments is tricky

- Process of fitting R-matrix to data can be difficult, time consuming and may not be reproducible
- The Atlas is rife with misclassified resonances!
- Often done with trial, error and significant human intervention

## Machine Learning approach

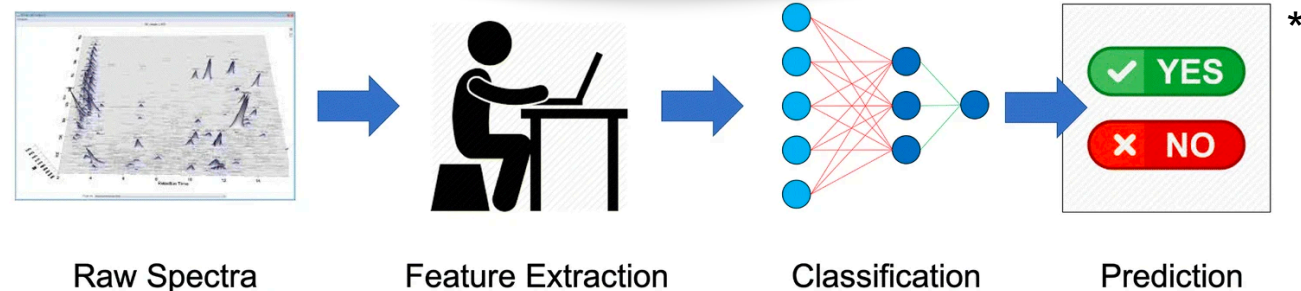




# Identifying resonance spin assignments is tricky

- Process of fitting R-matrix to data can be difficult, time consuming and may not be reproducible
- The Atlas is rife with misclassified resonances!
- Often done with trial, error and significant human intervention

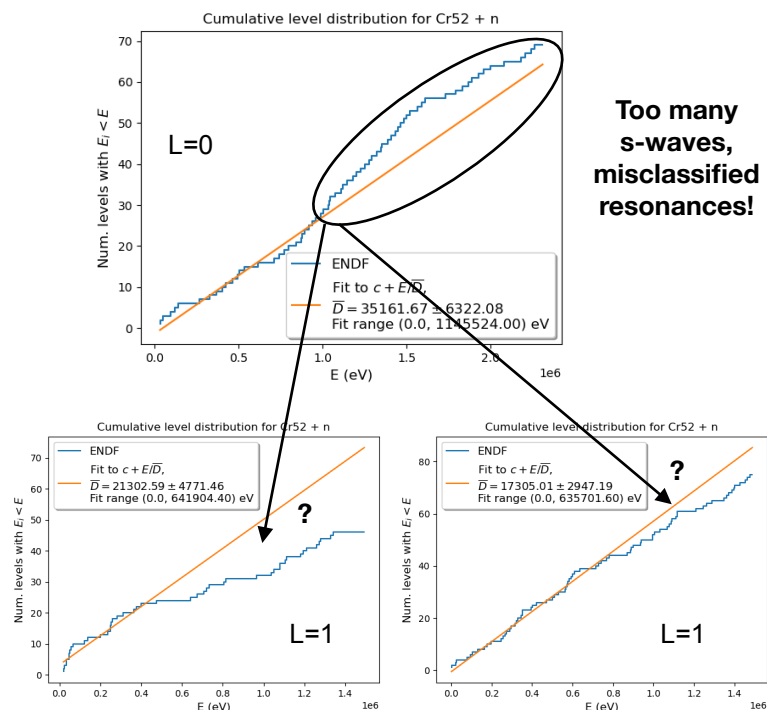
## Machine Learning approach



Lightweight scikit-learn classifiers + clever problem design may do the trick!

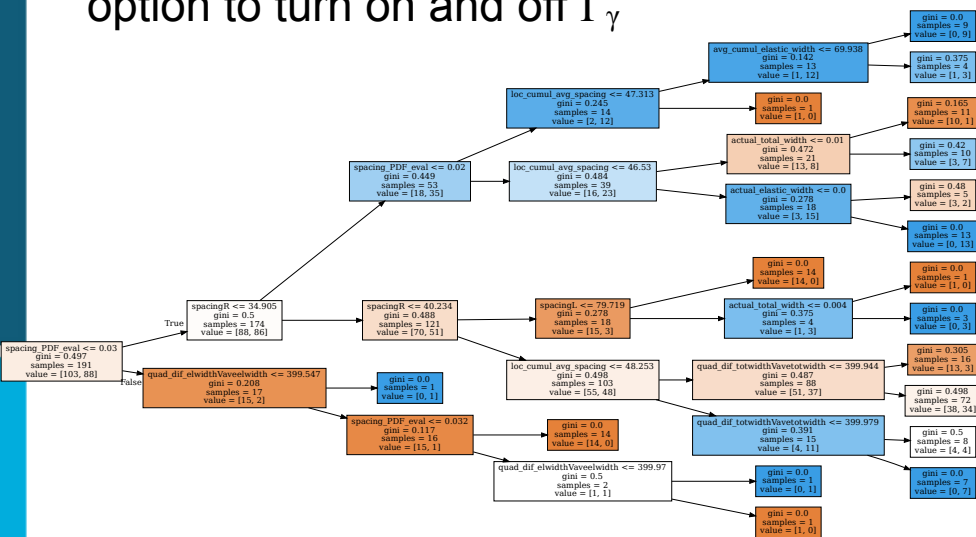
- Simple and robust method
- Convert resonances into features
- Cannot train and test on real data:
  - Synthetic resonances based on the statistical properties of real nuclei
  - “Jumble” these sequences to mimic mis-assignments
  - Split jumbled data into training and test sets
  - Assess accuracy of predictions
- Apply trained algorithm to sequence of real experimental data

\* Fig. taken from K.M. Mendez et al. *Metabolomics* 15, 142 (2019) <https://doi.org/10.1007/s11306-019-1608-0>



# Using SHAP to assess feature impact in classification

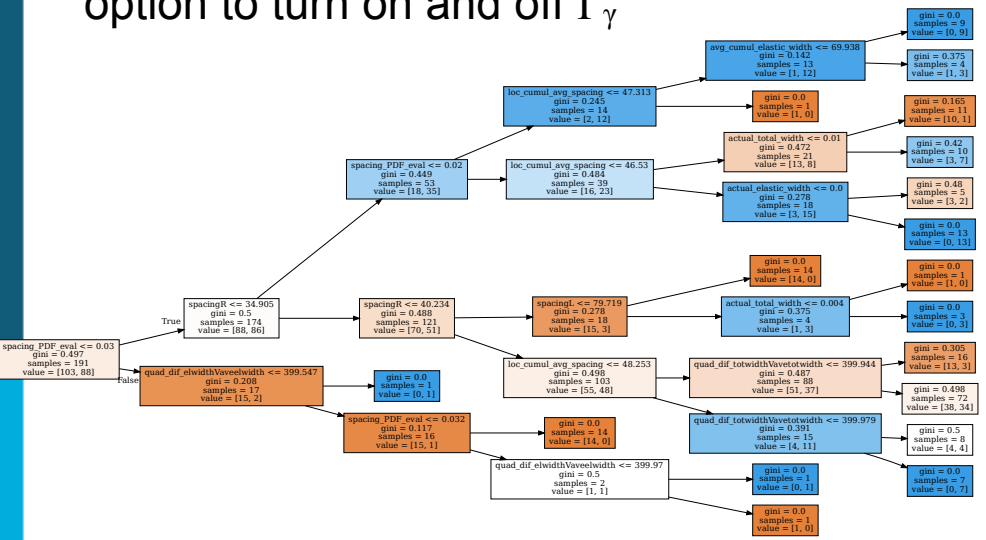
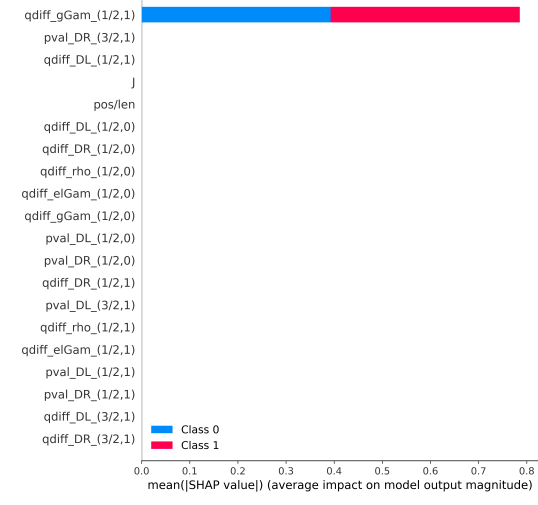
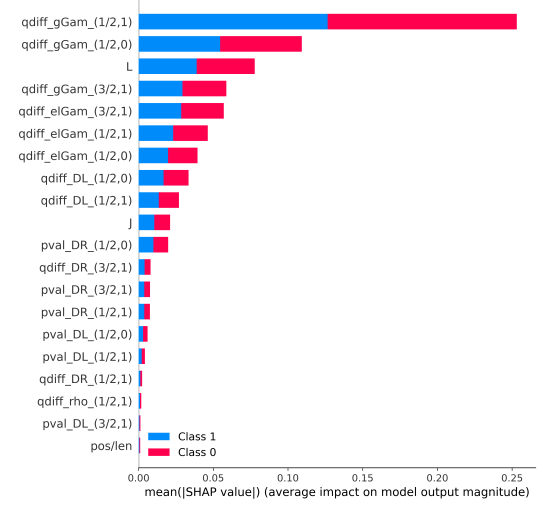
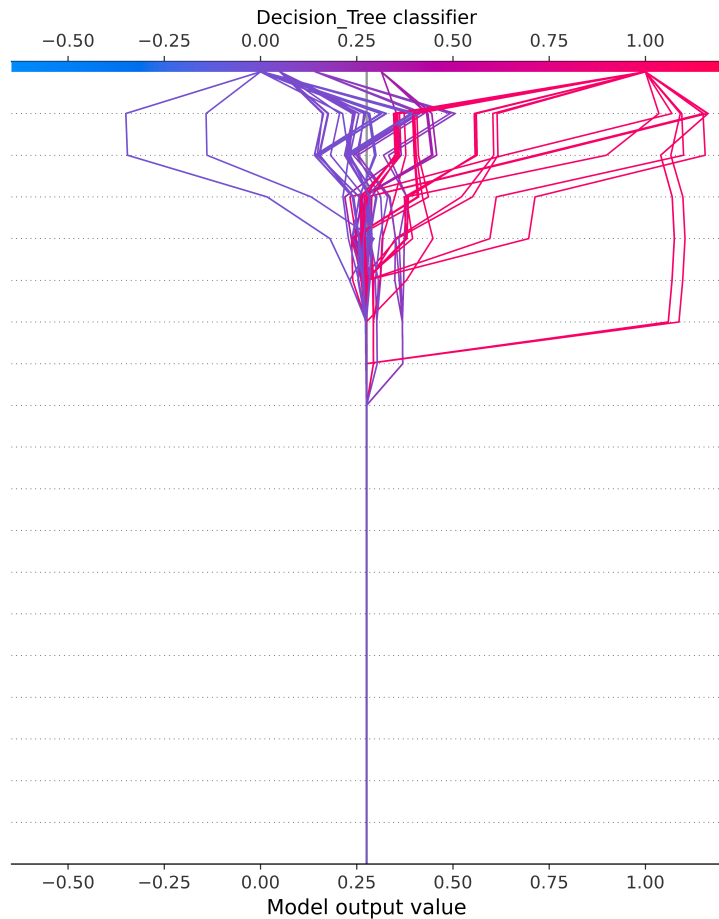
- Preliminary tests with an initial set of features using Decision Trees and Random Forests have shown signs of overfitting
- Used SHapley Additive exPlanations (SHAP) to quantify this
- Identified many unimportant features and an over-reliance on features related to  $\Gamma_\gamma$
- Redefined set of features and implemented option to turn on and off  $\Gamma_\gamma$



# Using SHAP to assess feature impact in classification

- Preliminary tests with an initial set of features using Decision Trees and Random Forests have shown signs of overfitting
- Used SHapley Additive exPlanations (SHAP) to quantify this
- Identified many unimportant features and an over-reliance on features related to  $\Gamma_\gamma$
- Redefined set of features and implemented option to turn on and off  $\Gamma_\gamma$

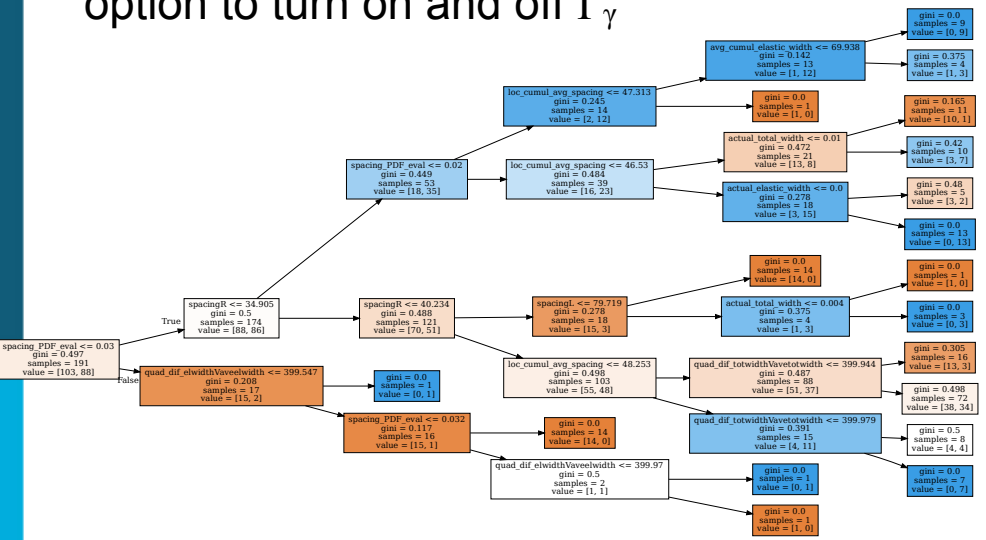
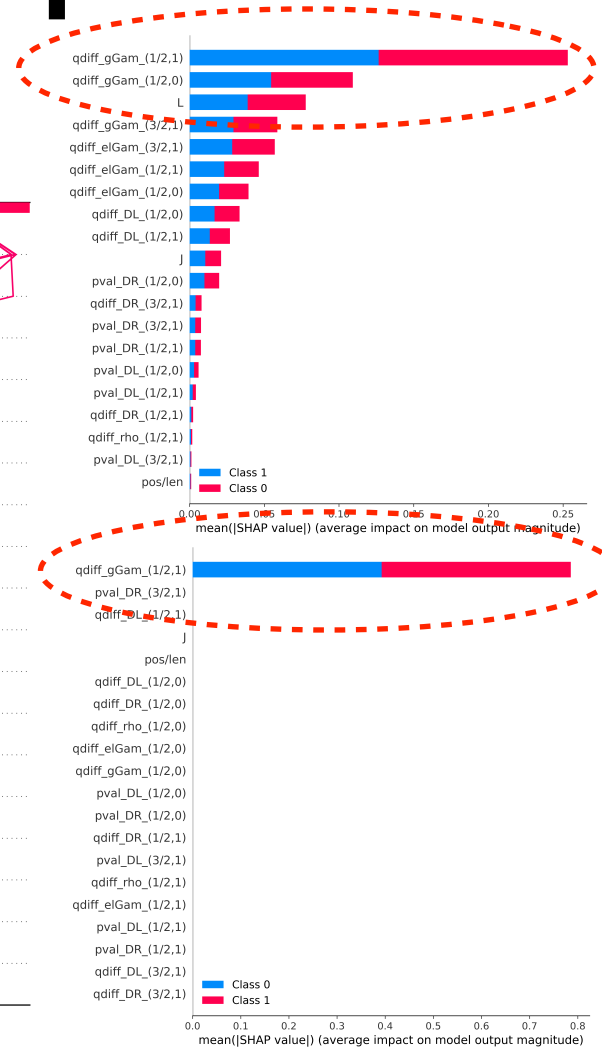
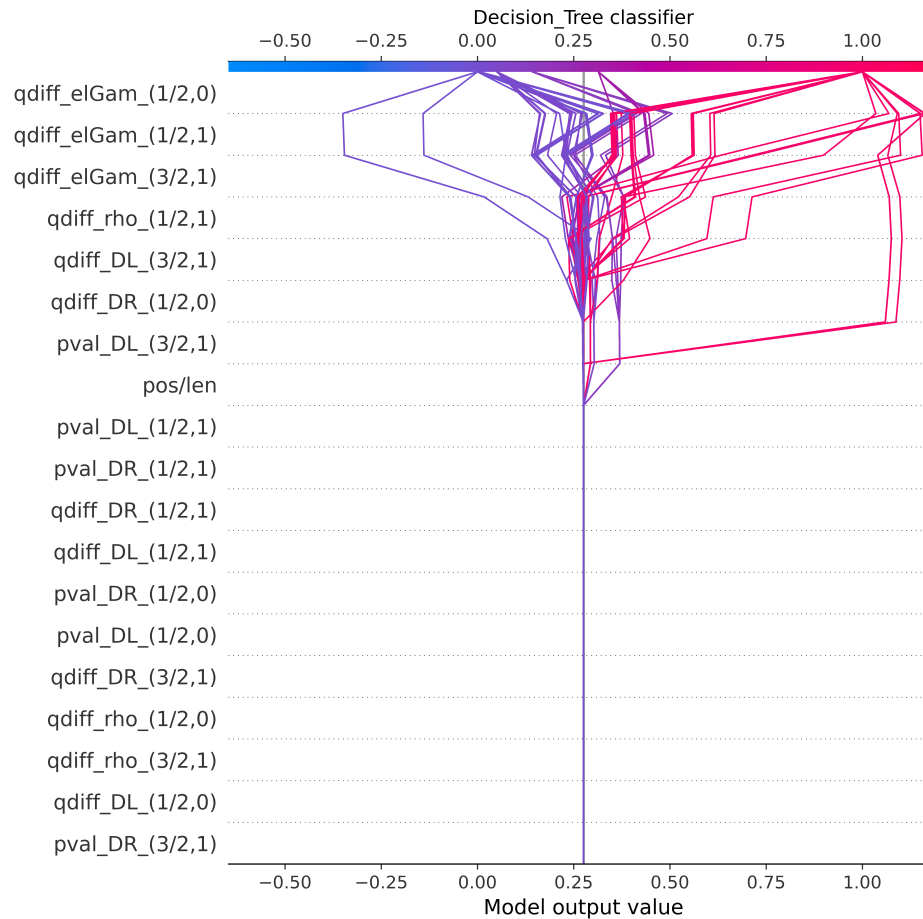
qdiff\_elGam\_(1/2,0)  
 qdiff\_elGam\_(1/2,1)  
 qdiff\_elGam\_(3/2,1)  
 qdiff\_rho\_(1/2,1)  
 qdiff\_DL\_(3/2,1)  
 qdiff\_DR\_(1/2,0)  
 pval\_DL\_(3/2,1)  
 pos/len  
 pval\_DL\_(1/2,1)  
 pval\_DR\_(1/2,1)  
 qdiff\_DR\_(1/2,1)  
 qdiff\_DL\_(1/2,1)  
 pval\_DR\_(1/2,0)  
 pval\_DL\_(1/2,0)  
 qdiff\_DR\_(3/2,1)  
 qdiff\_rho\_(1/2,0)  
 qdiff\_rho\_(3/2,1)  
 qdiff\_DL\_(1/2,0)  
 pval\_DR\_(3/2,1)





# Using SHAP to assess feature impact in classification

- Preliminary tests with an initial set of features using Decision Trees and Random Forests have shown signs of overfitting
- Used SHapley Additive exPlanations (SHAP) to quantify this
- Identified many unimportant features and an over-reliance on features related to  $\Gamma_\gamma$
- Redefined set of features and implemented option to turn on and off  $\Gamma_\gamma$



# Revised feature selection: Spacings & Widths

- **Spacings:**

- Use “signed p-value” of spacing relative to Wigner dist.
- If spacing too small, signal with minus sign (indicates resonance in wrong sequence)
- If spacing too big, indicates missing resonance

- **Test both spacing to left & right**

- GOE imposes short-long-short-long pattern
- Experiment with spacing-spacing correlation for same purpose

- **Elastic & Fission widths**

- Use diff to mean width as using Porter-Thomas leads to lower accuracy for small  $\nu$

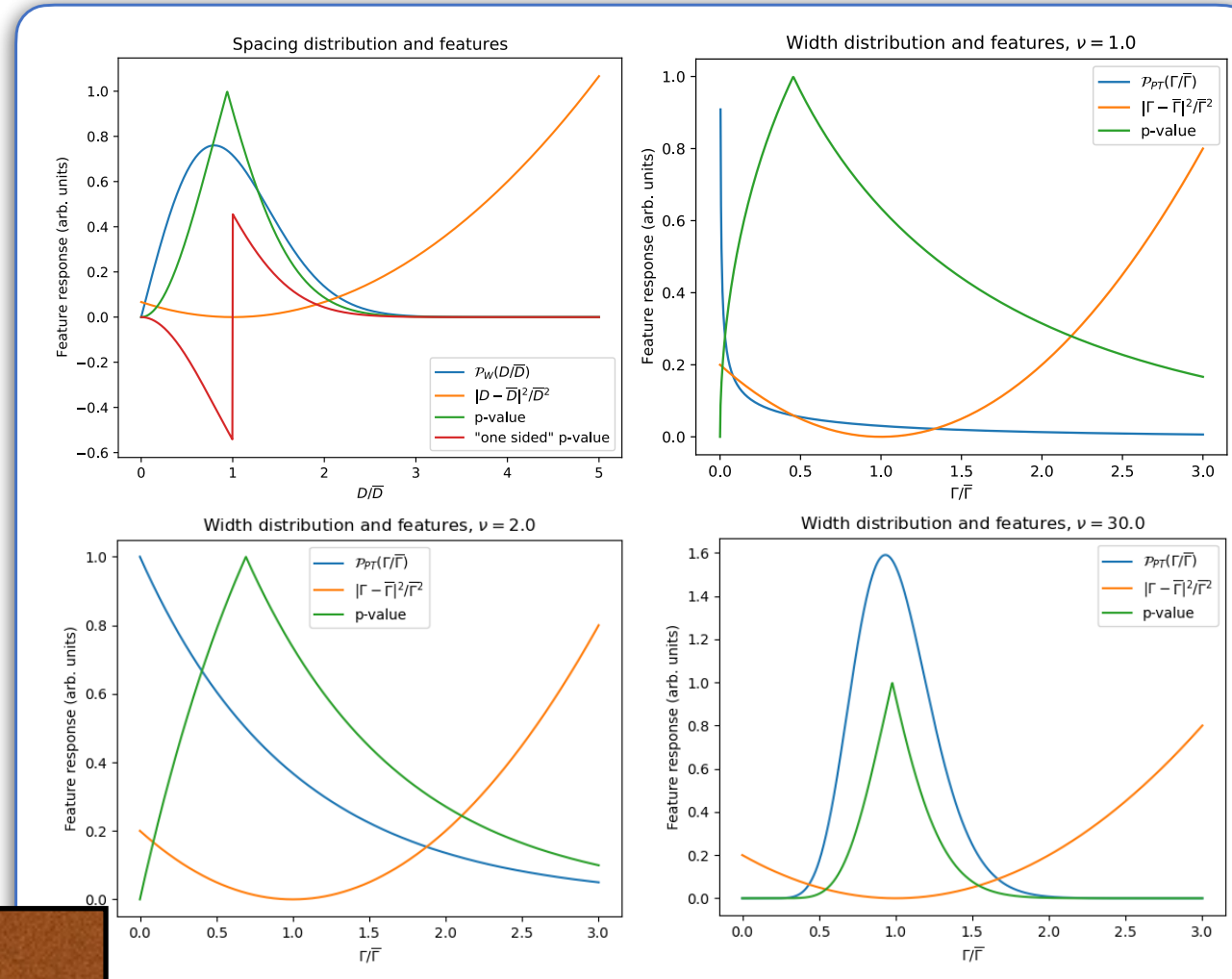
- **Don't use capture width by default as prone to exp. bias**

- **All features scaled to remove dependence on nucleus average parameters**

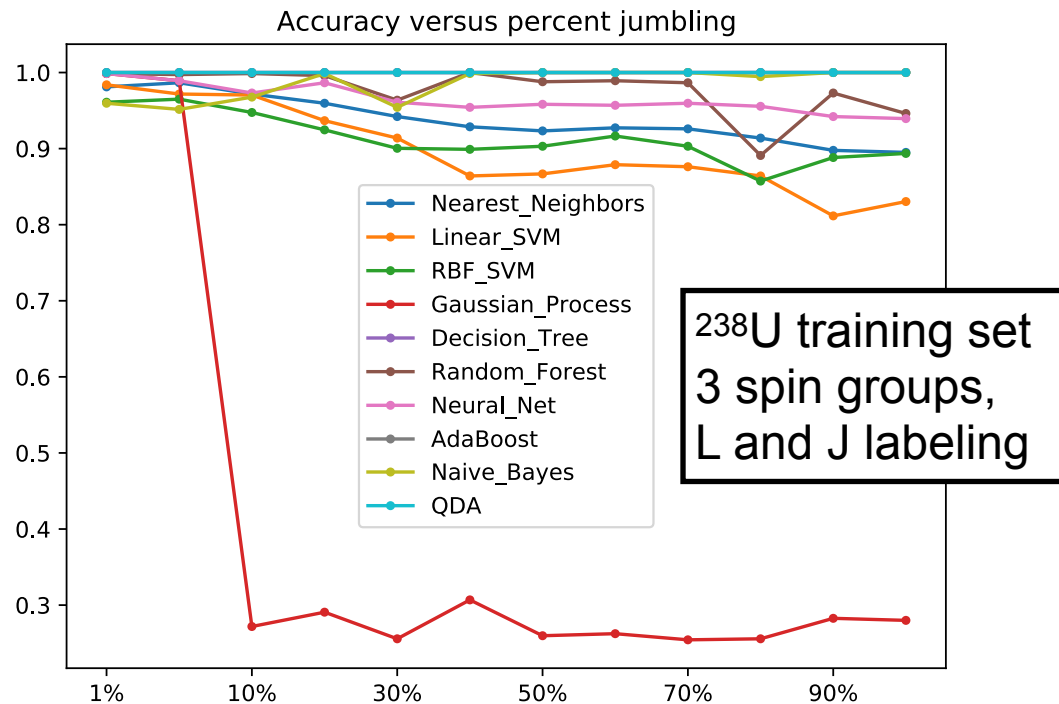
- **Use for all spingroups so can get signal for right/wrong assignments**

**Capture widths are dangerous:**

It is common for experimenter to specify width based on spin group assignment: Circular reasoning!



# Optimizing the training step

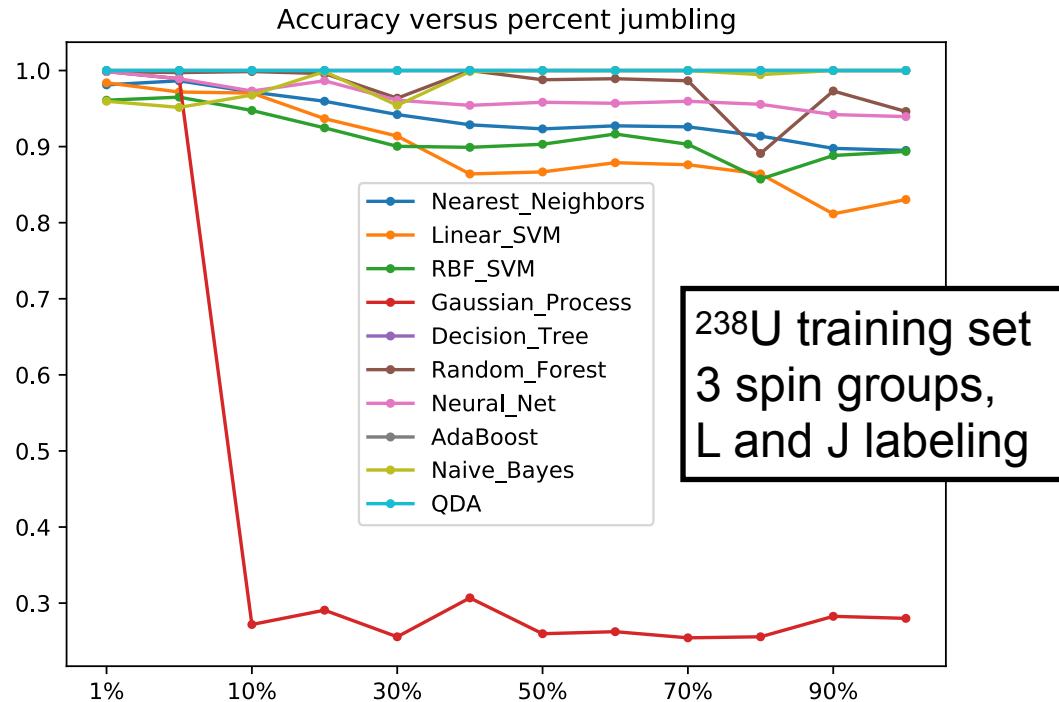


Default parametrization straight out of scikit-learn...

...we can do better!



# Optimizing the training step



Default parametrization straight out of scikit-learn...

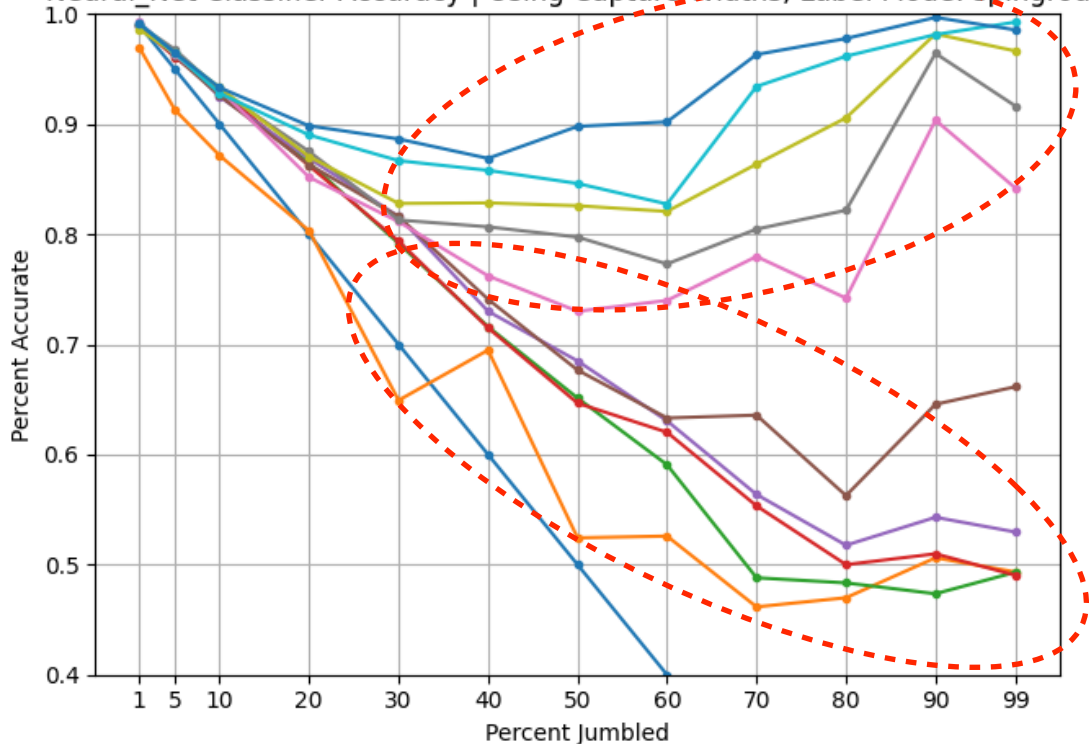
...we can do better!

- Grid search of hyper-parameters
- Began by varying the number of trees in a Random Forest
- Extended to ALL hyper-parameters for ALL classifiers in scikit-learn
- Did many runs so accuracies could be averaged
- Automated batch run to use the 400+ cores (144 dedicated to serial jobs) in the the NNDC computer cluster
- Ran with both  $\Gamma_\gamma$  feature on and off
- Classification by  $L$  and spin-group
- **SO MUCH** data that we're still processing them



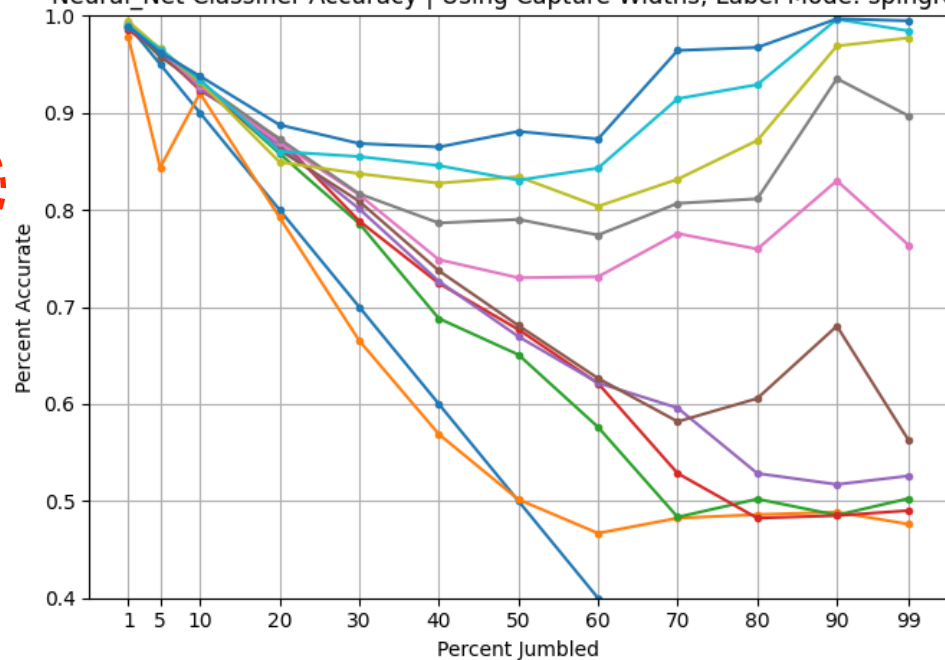
# Examples of the optimization results

Neural\_Net Classifier Accuracy | Using Capture Widths, Label Mode: spingroup



- No Classification
- alpha\_0.01\_max\_iter\_20\_hidden\_layer\_sizes\_20
- alpha\_0.01\_max\_iter\_20\_hidden\_layer\_sizes\_50
- alpha\_0.01\_max\_iter\_20\_hidden\_layer\_sizes\_100
- alpha\_0.01\_max\_iter\_20\_hidden\_layer\_sizes\_200
- alpha\_0.01\_max\_iter\_20\_hidden\_layer\_sizes\_500
- alpha\_0.01\_max\_iter\_200\_hidden\_layer\_sizes\_20
- alpha\_0.01\_max\_iter\_200\_hidden\_layer\_sizes\_50
- alpha\_0.01\_max\_iter\_200\_hidden\_layer\_sizes\_100
- alpha\_0.01\_max\_iter\_200\_hidden\_layer\_sizes\_200
- alpha\_0.01\_max\_iter\_200\_hidden\_layer\_sizes\_500

Neural\_Net Classifier Accuracy | Using Capture Widths, Label Mode: spingroup

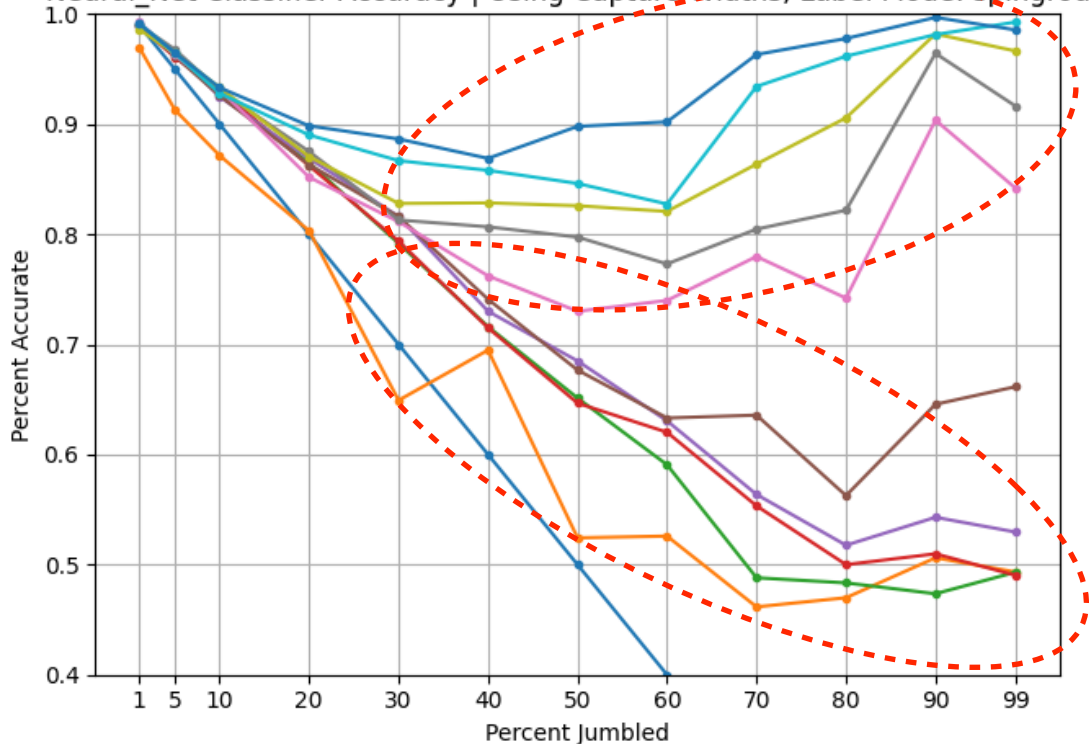


- No Classification
- alpha\_0.1\_max\_iter\_20\_hidden\_layer\_sizes\_20
- alpha\_0.1\_max\_iter\_20\_hidden\_layer\_sizes\_50
- alpha\_0.1\_max\_iter\_20\_hidden\_layer\_sizes\_100
- alpha\_0.1\_max\_iter\_20\_hidden\_layer\_sizes\_200
- alpha\_0.1\_max\_iter\_20\_hidden\_layer\_sizes\_500
- alpha\_0.1\_max\_iter\_200\_hidden\_layer\_sizes\_20
- alpha\_0.1\_max\_iter\_200\_hidden\_layer\_sizes\_50
- alpha\_0.1\_max\_iter\_200\_hidden\_layer\_sizes\_100
- alpha\_0.1\_max\_iter\_200\_hidden\_layer\_sizes\_200
- alpha\_0.1\_max\_iter\_200\_hidden\_layer\_sizes\_500



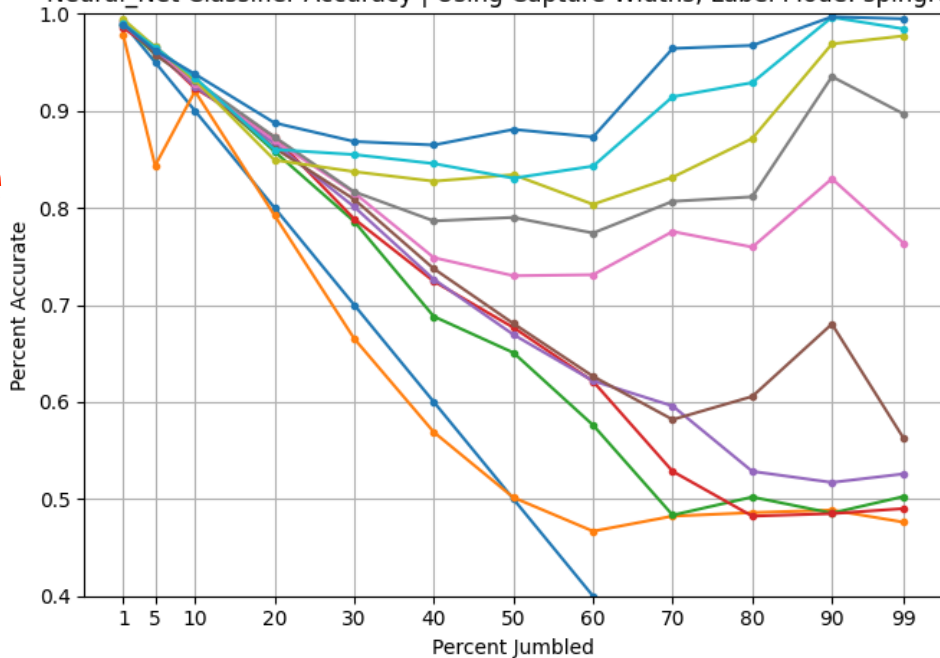
# Examples of the optimization results

Neural\_Net Classifier Accuracy | Using Capture Widths, Label Mode: spingroup



- No Classification
- alpha\_0.01\_max\_iter\_20\_hidden\_layer\_sizes\_20
- alpha\_0.01\_max\_iter\_20\_hidden\_layer\_sizes\_50
- alpha\_0.01\_max\_iter\_20\_hidden\_layer\_sizes\_100
- alpha\_0.01\_max\_iter\_20\_hidden\_layer\_sizes\_200
- alpha\_0.01\_max\_iter\_20\_hidden\_layer\_sizes\_500
- alpha\_0.01\_max\_iter\_200\_hidden\_layer\_sizes\_20
- alpha\_0.01\_max\_iter\_200\_hidden\_layer\_sizes\_50
- alpha\_0.01\_max\_iter\_200\_hidden\_layer\_sizes\_100
- alpha\_0.01\_max\_iter\_200\_hidden\_layer\_sizes\_200
- alpha\_0.01\_max\_iter\_200\_hidden\_layer\_sizes\_500

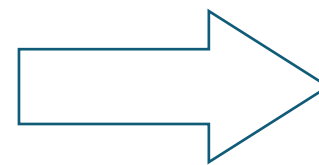
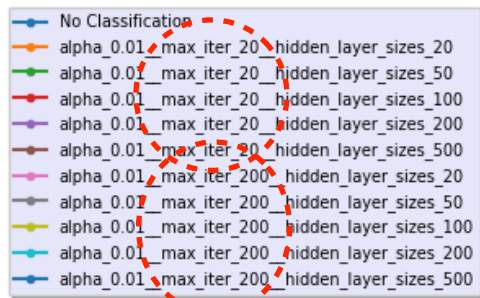
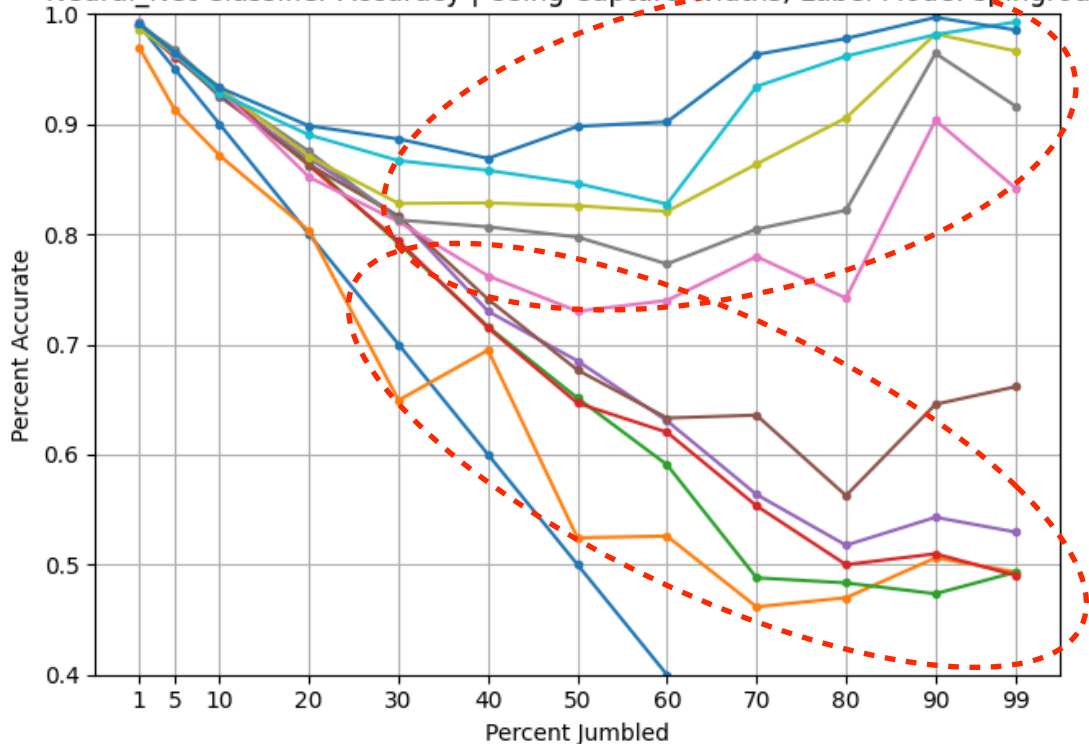
Neural\_Net Classifier Accuracy | Using Capture Widths, Label Mode: spingroup



- No Classification
- alpha\_0.1\_max\_iter\_20\_hidden\_layer\_sizes\_20
- alpha\_0.1\_max\_iter\_20\_hidden\_layer\_sizes\_50
- alpha\_0.1\_max\_iter\_20\_hidden\_layer\_sizes\_100
- alpha\_0.1\_max\_iter\_20\_hidden\_layer\_sizes\_200
- alpha\_0.1\_max\_iter\_20\_hidden\_layer\_sizes\_500
- alpha\_0.1\_max\_iter\_200\_hidden\_layer\_sizes\_20
- alpha\_0.1\_max\_iter\_200\_hidden\_layer\_sizes\_50
- alpha\_0.1\_max\_iter\_200\_hidden\_layer\_sizes\_100
- alpha\_0.1\_max\_iter\_200\_hidden\_layer\_sizes\_200
- alpha\_0.1\_max\_iter\_200\_hidden\_layer\_sizes\_500

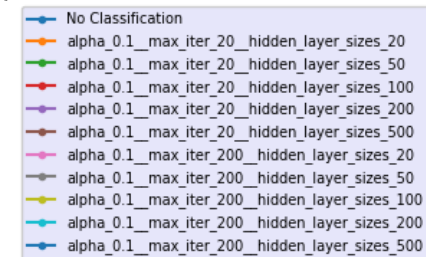
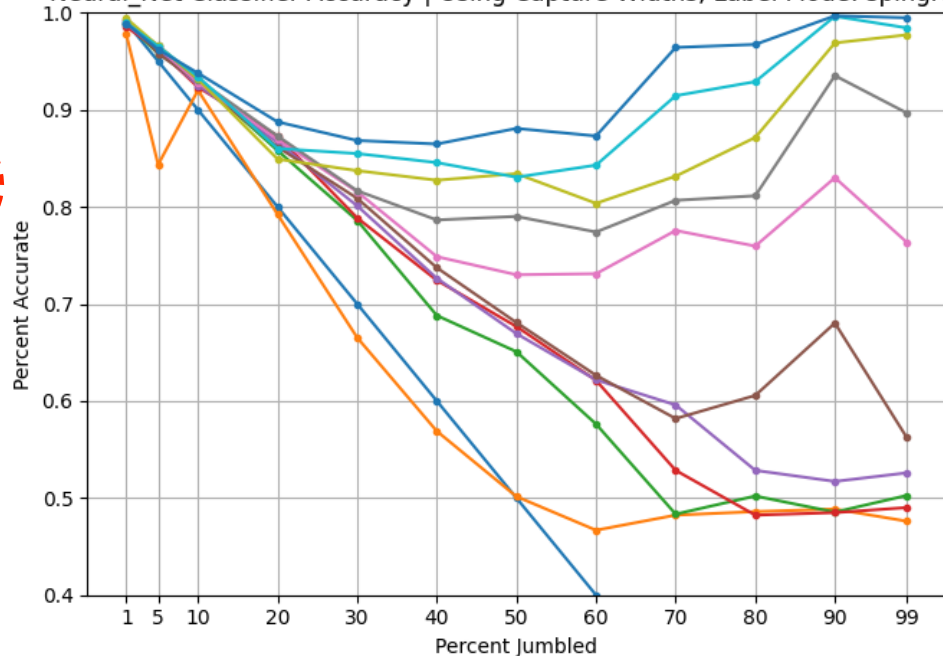
# Examples of the optimization results

Neural\_Net Classifier Accuracy | Using Capture Widths, Label Mode: spingroup



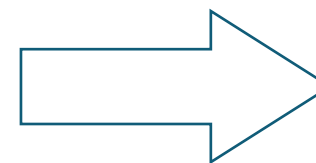
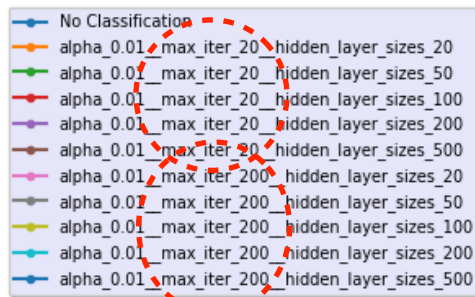
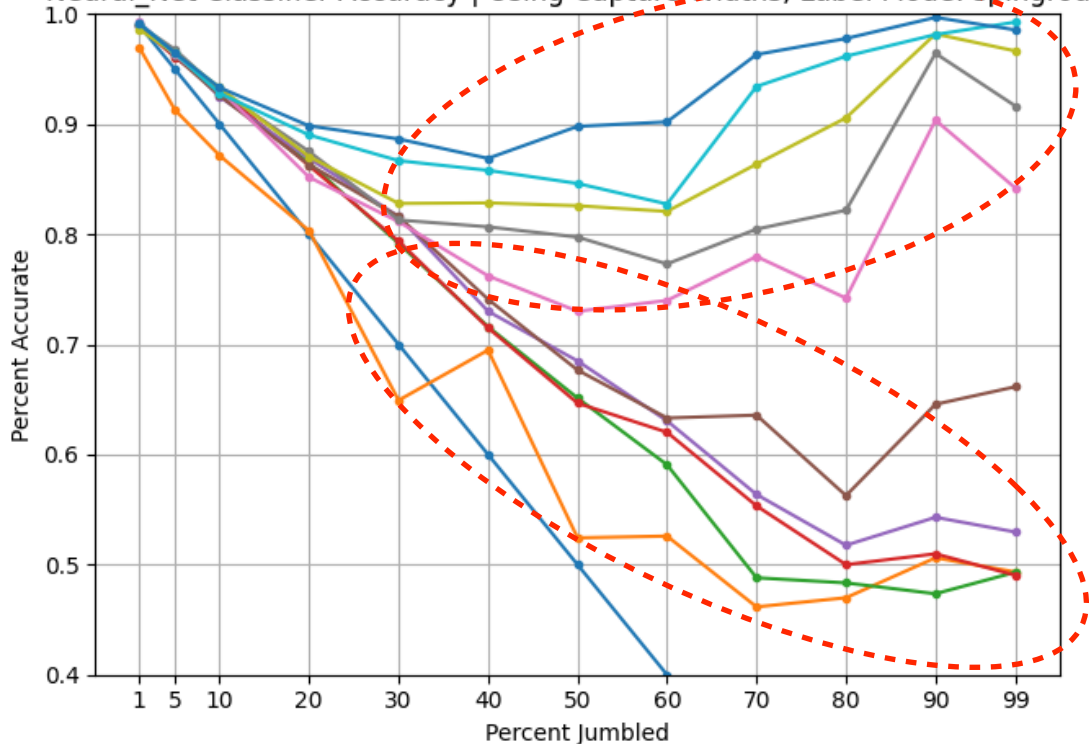
Maximum number of iterations makes significant impact!

Neural\_Net Classifier Accuracy | Using Capture Widths, Label Mode: spingroup



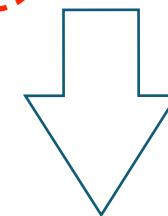
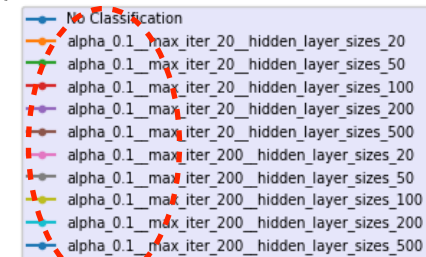
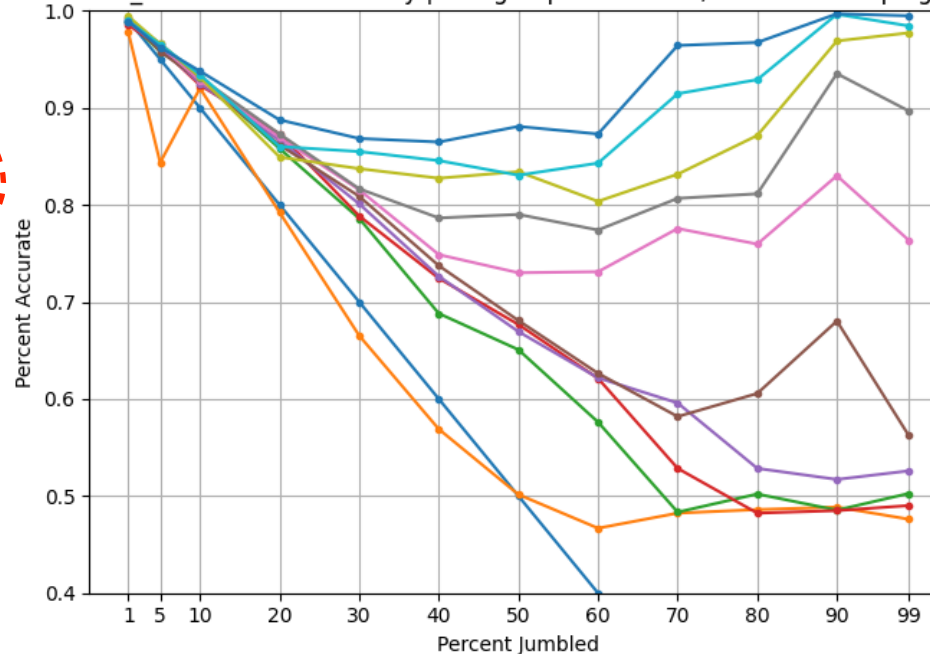
# Examples of the optimization results

Neural\_Net Classifier Accuracy | Using Capture Widths, Label Mode: spingroup



Maximum number of iterations makes significant impact!

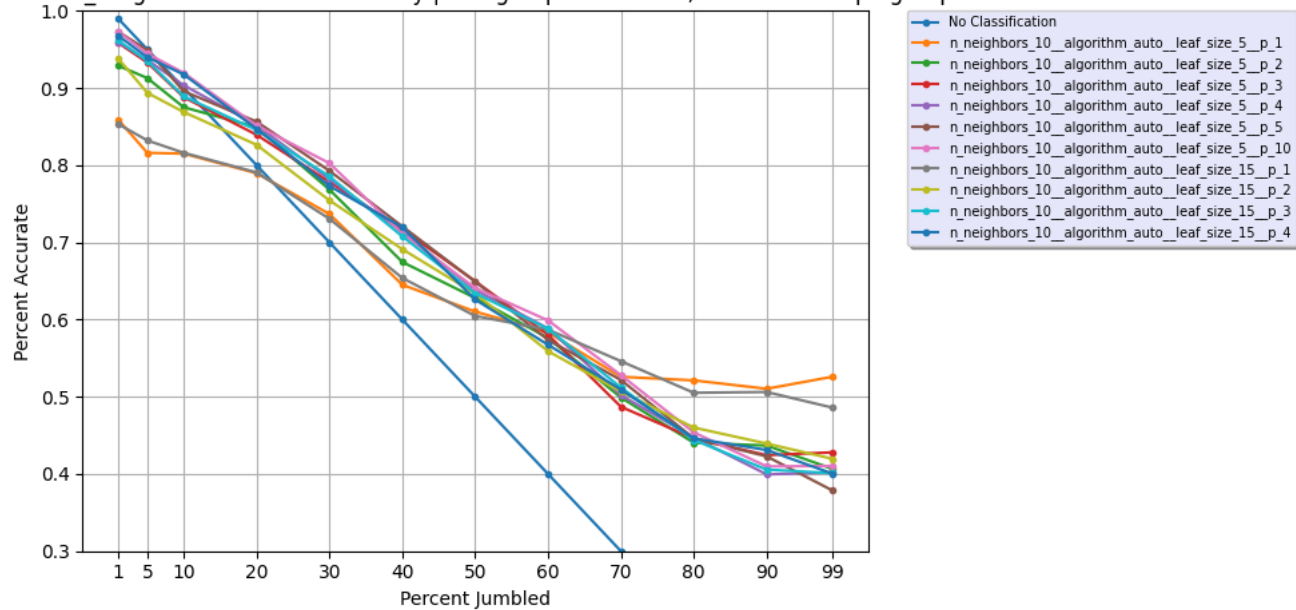
Neural\_Net Classifier Accuracy | Using Capture Widths, Label Mode: spingroup



Different regularizer, same conclusion

# Examples of the optimization results

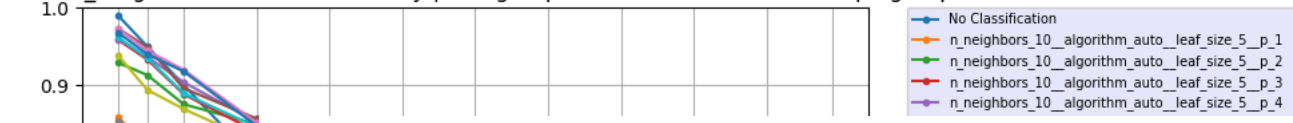
Nearest\_Neighbors Classifier Accuracy | Using Capture Widths, Label Mode: spingroup



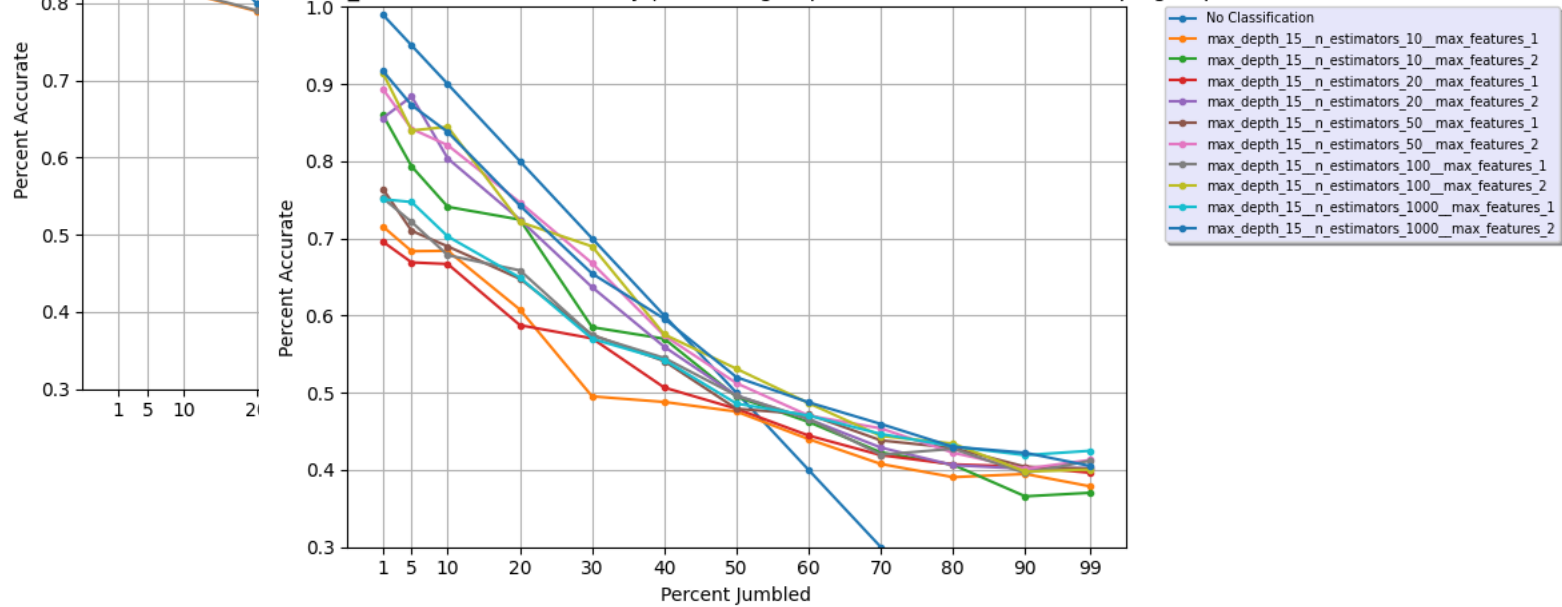


# Examples of the optimization results

Nearest\_Neighbors Classifier Accuracy | Using Capture Widths, Label Mode: spingroup

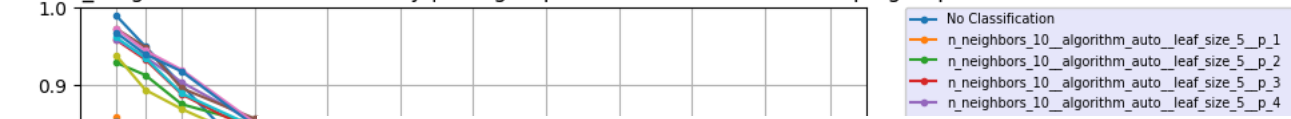


Random Forest Classifier Accuracy | Not Using Capture Widths, Label Mode: spingroup

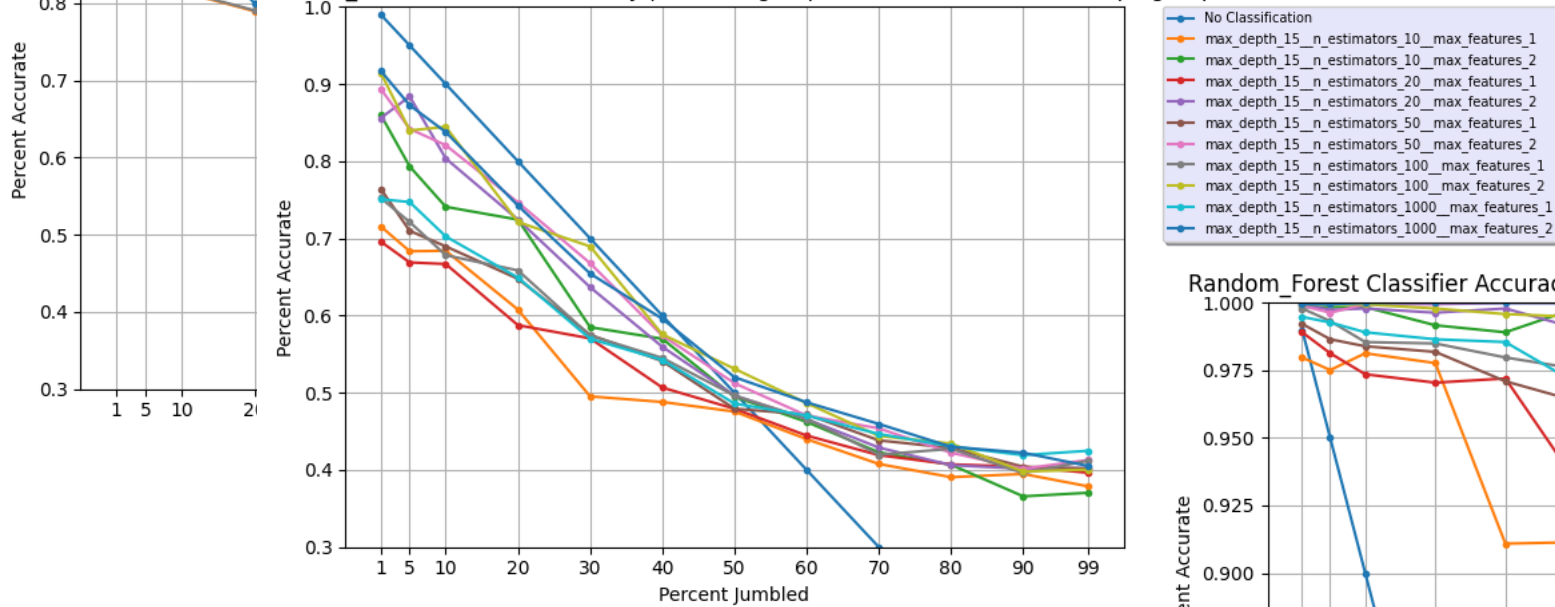


# Examples of the optimization results

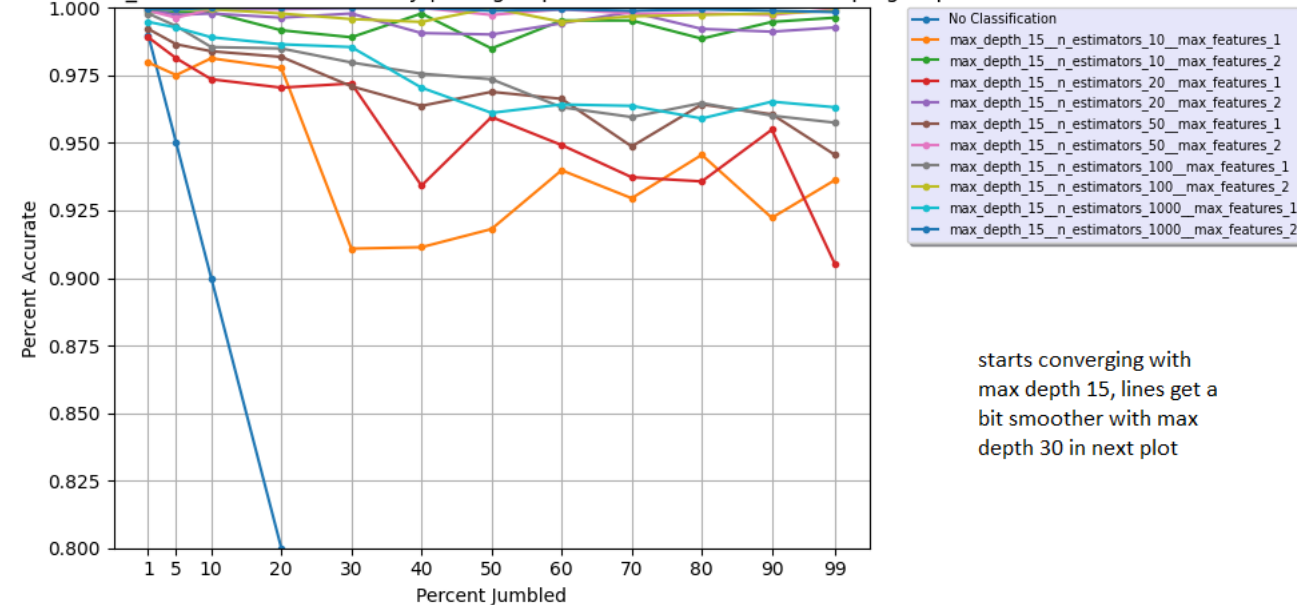
Nearest\_Neighbors Classifier Accuracy | Using Capture Widths, Label Mode: spingroup



Random\_Forest Classifier Accuracy | Not Using Capture Widths, Label Mode: spingroup



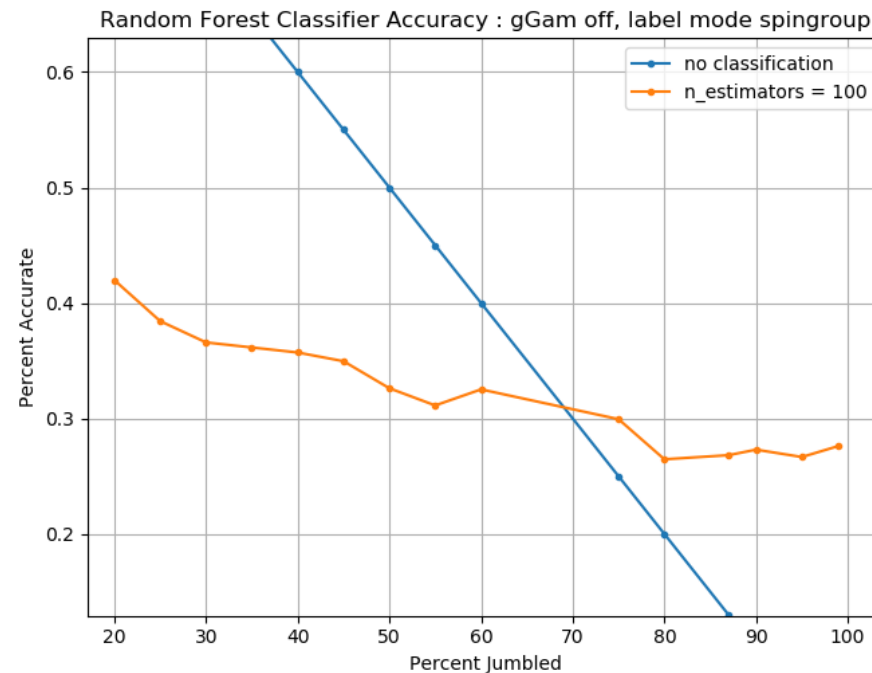
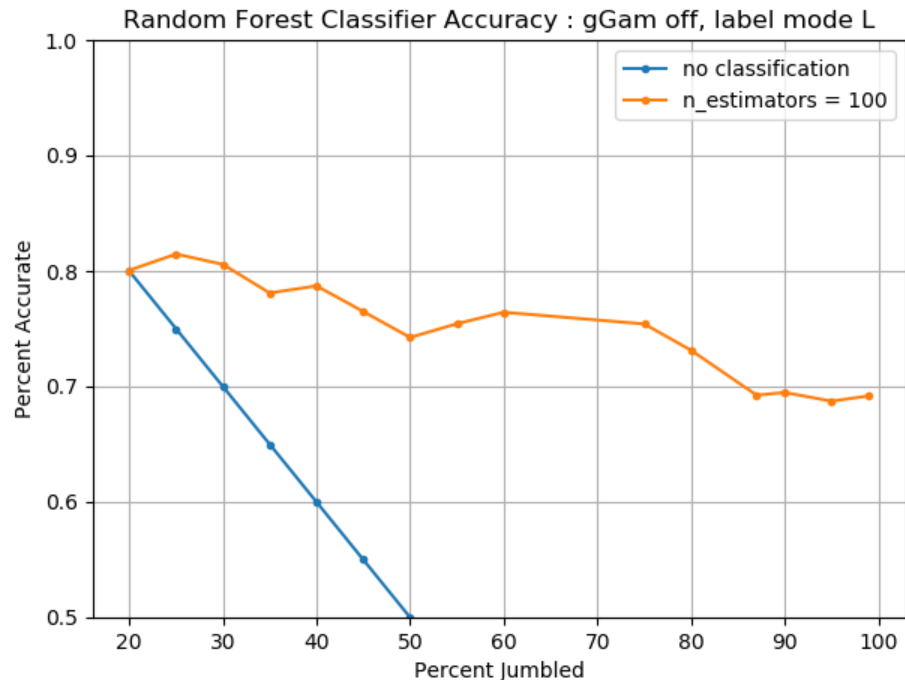
Random\_Forest Classifier Accuracy | Using Capture Widths, Label Mode: spingroup



starts converging with max depth 15, lines get a bit smoother with max depth 30 in next plot

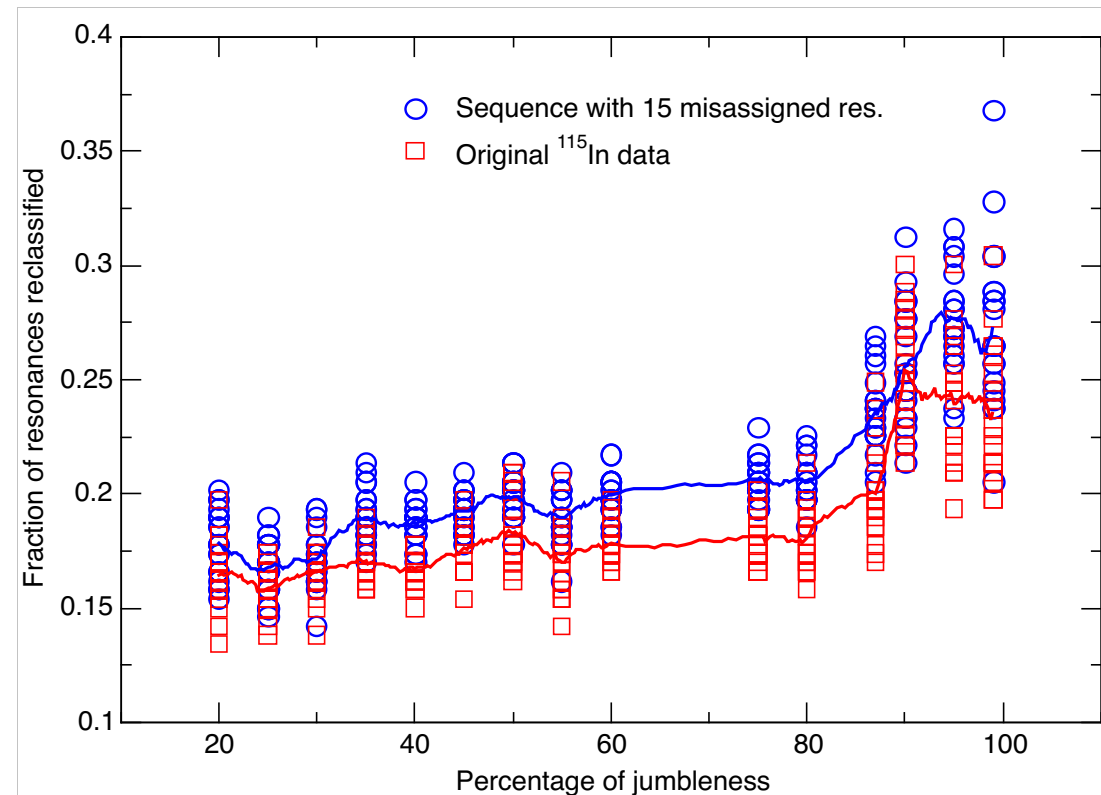
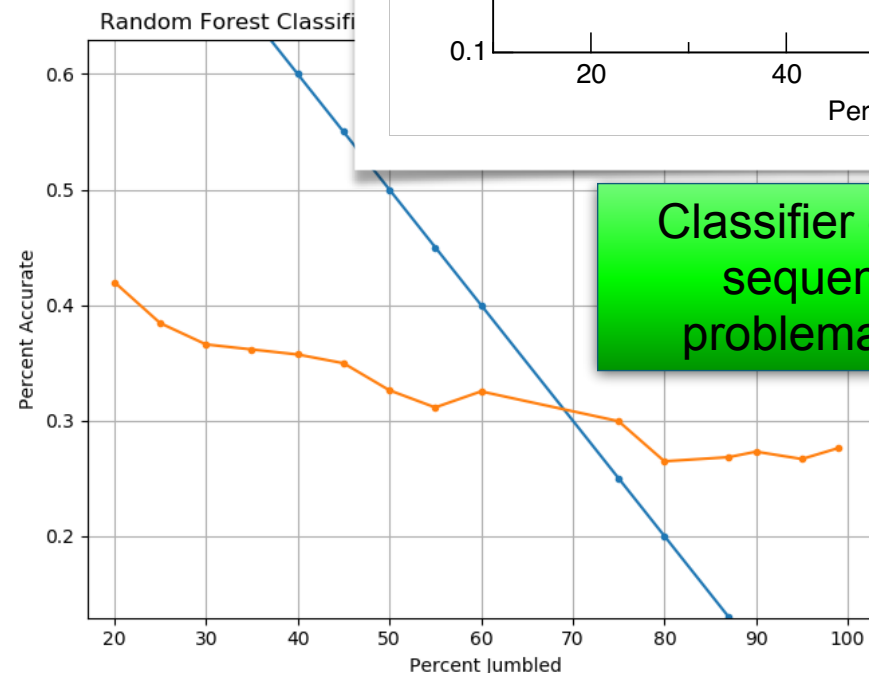
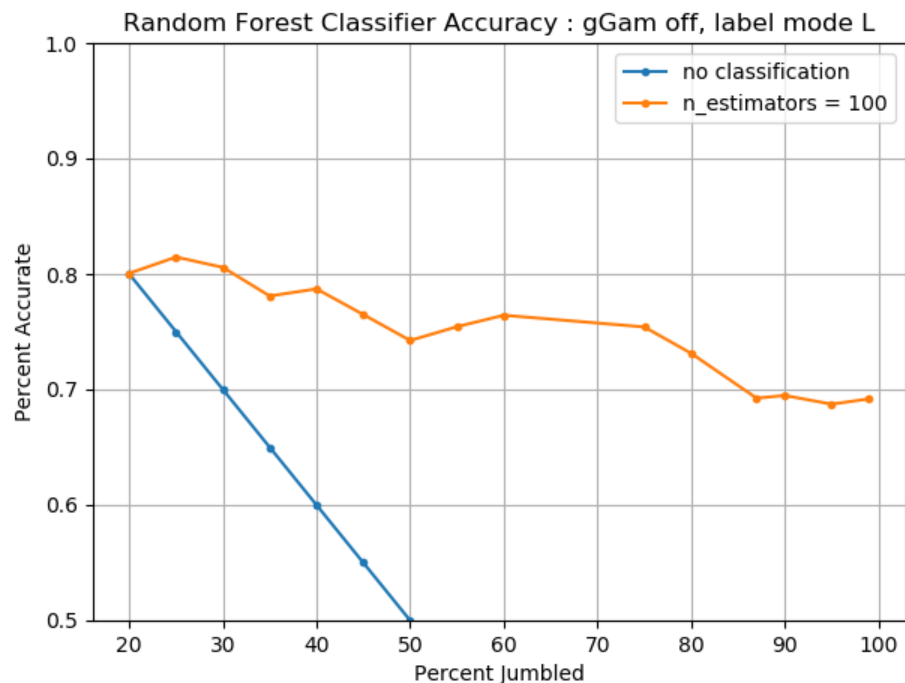
# Validating with polarized data - $^{115}\text{In}$

- Polarized-beam data offers more reliable information about the resonance spin
- We can use such data to validate our re-classification
- Out of many candidates, chose  $^{115}\text{In}$  (many points!)
- Purposefully misassigned some of the exp. resonances to investigate the behavior of the classifier



# Validating with polarized data - $^{115}\text{In}$

- Polarized-beam data offers more reliable information about the resonance spin
- We can use such data to validate our re-classification
- Out of many candidates, chose  $^{115}\text{In}$  (many points!)
- Purposefully misassigned some of the exp. resonances to investigate the behavior of the classifier



Classifier correctly detects sequence with more problematic resonances

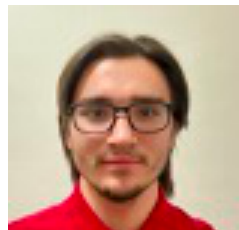


# Conclusion and future perspectives

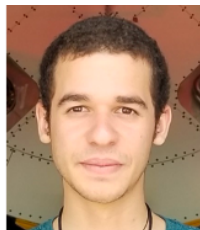
- We developed a Machine-Learning method to properly assign spins to neutron resonances: automated, general, reproducible
- Fully integrated with evaluated resonances in the Atlas: automation of new editions
- Transfer learning:
  - Train and optimize in synthetic data
  - Validate and deploy to real experimental resonances
- Very encouraging results!
- Will explore other classifiers and hyper-parameter combinations
- Will try to validate further with well-known nucleus (e.g.  $^{235}\text{U}$ )
- Thanks to all interns who worked and/or are collaborating on this project:



Sophia Hollick



Sergey Scoville



Pedro Rodriguez



Mary Fucci



Sergio Ruiz



Rose-Marie Crawford

# Acknowledgements

This work was supported by the Nuclear Criticality Safety Program, funded and managed by the National Nuclear Security Administration for the Department of Energy. Additionally, work at Brookhaven National Laboratory was sponsored by the Office of Nuclear Physics, Office of Science of the U.S. Department of Energy under Contract No. DE-AC02-98CH10886 with Brookhaven Science Associates, LLC. This project was supported in part by the Brookhaven National Laboratory (BNL), National Nuclear Data Center under the BNL Supplemental Undergraduate Research Program (SURP) and by the U.S. Department of Energy, Office of Science, Office of Workforce Development for Teachers and Scientists (WDTS) under the Science Undergraduate Laboratory Internships Program (SULI).